

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

## Model Results

**Predicted value:** 7.69e-12 cm<sup>3</sup>/molecule\*sec

**Global applicability domain:** Outside

**Local applicability domain index:** 2.04e-01

**Confidence level:** 7.69e-01

## Nearest Neighbors from the Training Set

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Dimethyl adipate

**Measured:** 8.40e-12

**Predicted:** 6.84e-12

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Dimethyl glutarate

**Measured:** 3.30e-12

**Predicted:** 3.76e-12

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Bornyl acetate

**Measured:** 1.39e-11

**Predicted:** 1.36e-11

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Cyclopropaneacetaldehyde, 2,2-dimethyl-3-(2-oxopropyl)-

**Measured:** 4.80e-11

**Predicted:** 4.73e-11

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Dimethyl succinate

**Measured:** 1.40e-12

**Predicted:** 1.93e-12